201-15171B

I U C L I D

D a t a S e t

Existing Chemical Substance ID: LABSA

Producer Related Part
Company: Compliance Services International
Creation date: 05-DEC-2000

Substance Related Part
Company: Compliance Services International
Creation date: 05-DEC-2000

Printing date: 30-JAN-2004
Revision date:
Date of last Update: **30-JAN-2004**

Number of Pages: **55**

Chapter (profile): Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile): Reliability: without reliability, 1, 2, 3, 4
Flags (profile): Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC

1.0.1 OECD and Company Information

Name: The LAB Sulfonic Acids Coalition

Remark: The Coalition consists of:

Colgate - Palmolive Company
Akzo Nobel Surface Chemistry LLC
The Dial Corporation
Stepan Company
Unilever HPC-USA

21-MAR-2003

1.0.2 Location of Production Site

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.0.3 Identity of Recipients

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.1 General Substance Information

Substance type: organic
Physical status: liquid
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (CAS# 68584-22-5)
Benzene sulfonic acid, dodecyl- (CAS# 27176-87-0)
Benzene sulfonic acid, tridecyl- (CAS# 25496-01-9)

21-JAN-2002

1.1.1 Spectra

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.2 Synonyms

Lauryl benzene sulfonic acid
29-JUN-2001

Alkylbenzene sulfonic acid
29-JUN-2001

Benzenesulfonic acid, C10-13-alkyl derivatives (CAS# 85536-14-7) [See assessment report for a discussion of the similarity between this European material and Benzene sulfonic acid, C10-16-alkyl derivatives (CAS# 68584-22-5)]
21-JAN-2002

Dodecyl benzene sulfonic acid
29-JUN-2001

Tridecyl benzene sulfonic acid
29-JUN-2001

1.3 Impurities

CAS-No:
EINECS-No:
EINECS-Name:
Remark: None
02-NOV-2001

1.4 Additives

CAS-No:
EINECS-No:
EINECS-Name:
Remark: None
02-NOV-2001

1.5 Quantity

Quantity 100 000 - 500 000 tonnes
05-NOV-2001

1.6.1 Labelling

Labelling:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.6.2 Classification

Classification:
Class of danger:
R-Phrases:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.7 Use Pattern

Type:
Category:
Remark: Primarily as an intermediate in the production of LAS.
02-NOV-2001

1.7.1 Technology Production/Use

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

1.8 Occupational Exposure Limit Values

Type of limit:
Limit value:
Remark: No TLV has been established
02-NOV-2001

1.9 Source of Exposure

Memo: No significant exposure. See discussion in accompanying LAB sulfonic acid assessment plan.
02-NOV-2001

1.10.1 Recommendations/Precautionary Measures

Remark: See LAB sulfonic acid assessment plan.
02-NOV-2001

1.10.2 Emergency Measures

Remark: See LAB sulfonic acid assessment plan.
02-NOV-2001

1.11 Packaging

Memo: Bulk transport

02-NOV-2001

1.12 Possib. of Rendering Subst. Harmless

Type of destruction:

Remark: Not applicable
02-NOV-2001

1.13 Statements Concerning Waste

Memo: See LAB sulfonic acid assessment plan.

02-NOV-2001

1.14.1 Water Pollution

Classified by:
Labelled by:
Class of danger:
Remark: Not a significant source of water pollution.
02-NOV-2001

1.14.2 Major Accident Hazards

Legislation:
Substance listed:
Remark: None
02-NOV-2001

1.14.3 Air Pollution

Classified by:
Labelled by:
Number:
Class of danger:
Remark: Not a significant source of air pollution.
02-NOV-2001

1.15 Additional Remarks

Memo: None
02-NOV-2001

1.16 Last Literature Search

Date of Search: 31-MAY-2001

02-JUL-2001

1.17 Reviews

Memo: None
02-NOV-2001

1.18 Listings e.g. Chemical Inventories

Remark: TSCA inventory (USA)
Domestic Substances List (DSL) - Canada
EINECS (Europe)
21-JAN-2002

2.1 Melting Point

Value: = -10 degree C
GLP: no
Remark: IUCLID cites source as Shell Chemicals U.K. Ltd. Chester
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Reliability: (2) valid with restrictions
21-FEB-2003 (27)

Value: < -10 degree C
GLP: no
Source: CONDEA Vista 1995.
Test substance: Alkylbenzene sulfonic acid with the following composition:

Components	CAS Number	Weight%
Nonylbenzenesulfonic Acid	35298-13-6	0.6
n-Decylbenzenesulfonic Acid	140-60-3	18.3
Undecylbenzenesulfonic Acid	50854-94-9	42.1
Dodecylbenzenesulfonic Acid	27176-87-0	30.0
Tridecylbenzenesulfonic Acid	25496-01-9	4.4
Tetradecylbenzenesulfonic Acid	30776-59-1	0.5
Sulfuric Acid	7664-93-9	1.3
Free Oil	None	2.4
Water	7732-18-5	0.4

Reliability: (4) not assignable
Data from Material Safety Data Sheet. No report available for review.
21-FEB-2003 (4)

Value: = 10 degree C
GLP: no data
Remark: Report not available but based on other sources this may actually be -10 degrees Celcius.
Source: Verschueren 1996.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
Peer-reviewed reference book.
21-FEB-2003 (80)

Value: = -10 degree C
GLP: no data
Remark: IUCLID cites source as Hoechst Iberica s.a. Barcelona.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
21-FEB-2003 (28)

Value: = 198.5 degree C
Decomposition: yes
Method: other: Thermal analysis was performed on the Netzsch DSC 204C and TG209C with N2 atmosphere.
GLP: no
Remark: This measured melting point value is significantly lower than the EPI Suite estimated values for other LAS materials. Decomposition onset at 444°C (47% weight loss at 500°C)
Source: Huntsman 2002.
Test substance: C10-14 Monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = C12.0. The test material is 85% active matter and is a coarse, cream-colored powder at 25°C.
Reliability: (2) valid with restrictions
21-FEB-2003 (23)

2.2 Boiling Point

Value: = 156 degree C
GLP: no
Source: CONDEA Vista 1995.
Test substance: Alkylbenzene sulfonic acid with the following composition:

Components	CAS Number	Weight%
Nonylbenzenesulfonic Acid	35298-13-6	0.6
n-Decylbenzenesulfonic Acid	140-60-3	18.3
Undecylbenzenesulfonic Acid	50854-94-9	42.1
Dodecylbenzenesulfonic Acid	27176-87-0	30.0
Tridecylbenzenesulfonic Acid	25496-01-9	4.4
Tetradecylbenzenesulfonic Acid	30776-59-1	0.5
Sulfuric Acid	7664-93-9	1.3
Free Oil	None	2.4
Water	7732-18-5	0.4

Reliability: (4) not assignable
Data from Material Safety Data Sheet. No report available for review.
21-FEB-2003 (4)

Value: = 315 degree C
GLP: no data
Source: Verschueren 1996.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
Peer-reviewed reference book.
21-FEB-2003 (80)

Value: = 205 degree C at 1013 hPa
Decomposition: no
GLP: no data
Remark: IUCLID cites source as Hoecht Iberica s.a. Barcelona.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
21-FEB-2003 (28)

Value:
Decomposition: yes
Method: other: Thermal analysis was performed on the Netzsch DSC 204C and TG209C with N2 atmosphere.
GLP: no
Remark: Decomposition onset at 444°C (47% weight loss at 500°C)
Source: Huntsman 2002.
Test substance: C10-14 monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = C12.0. The test material is 85% active matter and is a coarse, cream-colored powder at 25°C.
Reliability: (2) valid with restrictions
21-FEB-2003 (23)

2.3 Density

Type:
Value:
Remark: Not an HPV Challenge endpoint.
21-MAR-2003

2.3.1 Granulometry

Type of distribution:

Remark: Not an HPV Challenge endpoint.
21-MAR-2003

2.4 Vapor Pressure

Value: = 2.89 x 10^{-8} Pa
GLP: no
Source: EPA 2000
Test substance: Benzene sulfonic acid, undecyl (50854-94-9), which is closest to the low end of the actual alkyl chain length (11.3-11.8) of Benzene sulfonic acid, C10-16 alkyl derivatives (68584-22-5)
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
6-JAN-2004 (76)

Value: = 1.06 x 10^{-8} Pa
GLP: no
Source: EPA 2000
Test substance: Benzenesulfonic acid, dodecyl (CAS#27176-87-0); C12 was used in the EPI Suite modeling - the actual average range of alkyl chain lengths for dodecyl benzenesulfonic acid is 11.3-12.6
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
6-JAN-2004 (76)

Value: = 3.85 x 10^{-9} Pa
GLP: no
Source: EPA 2000
Test substance: Benzenesulfonic acid, tridecyl (CAS#25496-01-9); C13 was used in the EPI Suite modeling - the actual average range of alkyl chain lengths for tridecyl benzenesulfonic acid is 11.8-12.6
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
6-JAN-2004 (76)

Value: = 0 hPa
Method: other (calculated)
Remark: The reported value is 3x10-13 Pa.
Cites estimates calculated by Lyman (see References).
Source: HERA 2002; Lyman 1985.
Test substance: C12 LAS (CAS #25155-30-0)
Reliability: (4) not assignable
21-FEB-2003 (18) (43)

2.5 Partition Coefficient

log Pow: = 2 at 23 degree C
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year: 1981
GLP: no
Remark: IUCLID cites source as Shell Chemical U.K. Ltd. Chester. No report available for review.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Reliability: (2) valid with restrictions
05-DEC-2001 (27)

log Pow: = 1.96
Method: other (calculated): Leo and Hansch
Year: 1971
GLP: no data
Remark: Original data from Leo, A., Hansch, C., and Elkins, D. 1971. Chem. Rev. 71:525-616.
Source: Hand and Williams 1987.
Test substance: Sodium dodecylbenzenesulfonate as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
Based on data from standard reference source.
11-OCT-2001 (16)

log Pow: = 2.52
Method: other (calculated): Leo and Hansch
Year: 1971
GLP: no data
Remark: Original data from Leo, A., Hansch, C., and Elkins, D. 1971. Chem. Rev. 71:525-616.
Source: Hand and Williams 1987.
Test substance: Sodium tridecylbenzene sulfonate as surrogate for benzene sulfonic acid, tridecyl- (25496-01-9)
Reliability: (2) valid with restrictions
Based on data from standard reference source.
11-OCT-2001 (16)

log Pow: = 3.32
Method: other (calculated)
Year:
GLP: no
Remark: Calculated using the method of Leo and Hansch (1979) modified to take into account the various phenyl positions along the linear alkyl chain as per Roberts (1991).
Source: HERA 2002; Roberts 1991; Leo and Hansch 1979.
Test substance: C11.6 LAS
Reliability: (4) not assignable
21-FEB-2003 (18) (39) (65)

2.6.1 Water Solubility

Value: 400000 mg/l at 20 degree C
GLP: no
Remark: The IUCLID Data Sheet cites a Shell Chemical report indicating that the substance is miscible in water up to 40%.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Reliability: (2) valid with restrictions
05-DEC-2001 (27)

Value: = 300000 mg/l at 20 degree C
pH: > 9
GLP: no data
Remark: The IUCLID Data Sheet cites a Shell Chemical report indicating that the substance is miscible in water up to 40%.
Source: IUCLID 1995.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0)
Reliability: (2) valid with restrictions
04-DEC-2001 (28)

Result: The reported pKa for all of the LAB sulfonic acids is < 1.
Source: Noeller 1966; Lide 1990.
Test substance: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5), Benzene sulfonic acid, dodecyl- (27176-87-0), and Benzene sulfonic acid, tridecyl- (25496-01-9)
Reliability: (2) valid with restrictions
11-OCT-2001 (40) (50)

Value: > 250 g/l
Qualitative: miscible
GLP: no data
Remark: The study shows that 25% solutions (250 g/L) of various LASs have cloud clear points (i.e., form clear solutions) at temperatures of 2-21°C or above. Therefore, the results demonstrate that 25% solutions of LAS are soluble at room temperature. LAS has a critical micelle concentration (CMC) value of 0.1 mg/L.
Source: Cohen 1995.
Test substance: Various LASs made from four commercial LABs, average alkyl chain length = 11.6
Reliability: (2) valid with restrictions
21-FEB-2003 (3)

pH: = 10
GLP: no data
Remark: Reported pH value is 10.0 +/- 1.0 (1% solution).
Source: Huntsman 2002.
Test substance: C10-14 monoalkylbenzene sulfonic acid, sodium salt (CAS #85117-50-6); mean molecular weight = 348, average alkyl chain length = C12.0
Reliability: (4) not assignable
21-FEB-2003 (22)

2.6.2 Surface Tension

Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.7 Flash Point

Value:
Type:
Method:
Year:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.8 Auto Flammability

Value:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.9 Flammability

Result:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.10 Explosive Properties

Result:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.11 Oxidizing Properties

Result:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

2.12 Additional Remarks

Memo: None
11-OCT-2001

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001352 cm3/(molecule * sec)
Degradation: = 50 % after 8.6 hour(s)
Method: other (calculated): EPISuite, Version 3.10
Year: **GLP:**
Test substance:
Source: USEPA 2000.
Test substance: Benzene sulfonic acid, undecyl (50854-94-9) as a surrogate for Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5). The C11 sulfonic acid was used because it more closely approximates the average alkyl chain length for the C10-16 material, which ranges from 11.0 to 11.8. The EpiSuite model calculates the C10-16 material based on its lowest alkyl chain length, which is C10. This half-life value was 9.5 hours.
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
21-JAN-2002 (76)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001636 cm3/(molecule * sec)
Degradation: = 50 % after 7.9 hour(s)
Method: other (calculated): EPISuite, Version 3.10
Year: **GLP:**
Test substance: other TS: Benzene sulfonic acid, dodecyl (27176-87-0). The EPISuite model calculates this material based on a C12 alkyl chain length rather than the full range of carbon chain lengths present.
Source: USEPA 2000.
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
21-JAN-2002 (76)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001777 cm3/(molecule * sec)
Degradation: = 50 % after 7.2 hour(s)
Method: other (calculated): EPISuite, Version 3.10
Year: **GLP:**
Test substance: other TS: Benzene sulfonic acid, tridecyl (25496-01-9). The EPISuite model calculates this material based on a C13 alkyl chain length rather than the full range of carbon chain lengths present.
Source: USEPA 2000.
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
21-JAN-2002 (76)

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1500000 molecule/cm3
Rate constant: = .00000000001339 cm3/(molecule * sec)
Degradation: = 50 % after 7.9 hour(s)
Method: other (calculated): EPISuite, Version 3.10
Year: **GLP:**
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (25155-30-0 et al.). The modeled material was a C12-LAS.
Source: USEPA 2000.
Reliability: (2) valid with restrictions
Standard peer-reviewed database and estimation software.
21-JAN-2002 (76)

Type: water
Light source: other: Mercury vapor lamp
Light spect.: = 200 - 350 nm
DIRECT PHOTOLYSIS
Degradation: > 95 % after 20 minute(s)
Method:
Year: **GLP:** no data
Test substance: other TS: LAS; activity: 95% (CAS #25155-30-0)
Method: A series of photodegradation studies were conducted. Aqueous solution of LAS (pH 6.75) were passed through an irradiated tubular flow reactor. Reaction rates were obtained for both non-sensitized conditions and when ferric perchlorate (0.04 to 3.15 x 10-4 g-mole/L) was used as a sensitizer. A Hanovia 1200-watt mercury-vapor lamp was the source of radiation. The LAS concentration was determined by the methylene blue method.
Remark: Rapid photodegradation occurred in indirect photolysis degradation. Complete conversion of LAS to intermediates at an average residence time as low as 1 minute. The maximum conversion to CO2 was obtained at a residence time of 20 minutes and corresponded to 7 moles CO2 per mole of LAS. Reaction rate increases by two orders of magnitude in presence of ferric perchlorate. Half order kinetics with respect to

light intensity and LAS concentration explained the data for nonsensitized conditions. An appropriate rate equation could be derived by assuming a second-order deactivation of light-activated LAS molecules. The sensitized reaction was believed to occur by abstraction of hydrogen atoms from LAS by hydroxyl radicals. Hydroxyl radicals presumably are produced by an electron-transfer reaction involving light-activated ferric ions. The mechanism is complex; over-all kinetics indicated a first-order effect of (Fe+3), 1.2 order in light intensity, and maxima in the rate for intermediate LAS and O2 concentrations.

Initial LAS concentration was 60 to 182 mg/L.

Source: Matsuura and Smith 1970.
Reliability: (2) valid with restrictions
20-FEB-2003 (45)

3.1.2 Stability in Water

Type: abiotic
Method:
Year: **GLP:** no data
Test substance: other TS: C10-13 alkylbenzene sulfonic acid, sodium salt (CAS #68411-30-3)
Remark: LAS is stable in water. LAS can be decomposed at extreme conditions such as elevated temperatures in the presence of inorganic acids such as phosphoric, sulphuric and hydrochloric acid, e.g.: 60-70% sulphuric acid at 140 - 190 degree C or with concentrated HCl in a sealed container at 150 - 200 degree C. Information as cited in IUCLID Data Sheet for CAS #68411-30-3.
Source: Cross and Dekker 1977.
Reliability: (4) not assignable
21-FEB-2003 (5)

3.1.3 Stability in Soil

Type: **Radiolabel:**
Concentration:
Cation exch. capac.
Microbial biomass:
Method:
Year: **GLP:**
Test substance:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

3.2 Monitoring Data (Environment)

Type of measurement:
Medium:
Remark: None
02-NOV-2001

3.3.1 Transport between Environmental Compartments

Type:
Media:
Method:
Year:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

3.3.2 Distribution

Method: other (calculation): Fugacity Level III
Remark: Mass Distribution by Environmental Compartment

Air: 1.13%
Water: 31.7%
Soil: 63.3%
Sediment: 3.81%

Source: USEPA 2000.
Test substance: Benzene sulfonic acid, undecyl (50854-94-9), which is closest to the low end of the actual alkyl chain length (11.3-11.8) of Benzene sulfonic acid, C10-16 alkyl derivatives (68584-22-5)
Remarks: EPI Suite utilizes input values for relevant physicochemical parameters from its resident database, which has undergone extensive peer review and is accessed by input of the CAS number.
Reliability: (2) valid with restrictions
21-JAN-2002 (76)

Method: other (calculation): Fugacity Level III
Remark: Mass Distribution by Environmental Compartment

Air: 1.03%
Water: 29.1%
Soil: 59.7%
Sediment: 10.0%

Source: USEPA 2000.
Test substance: Benzene sulfonic acid, dodecyl- (27176-87-0); C12 was used in the EPI Suite modeling - the actual average range of alkyl chain lengths for dodecyl benzenesulfonic acid is 11.3-12.6
Remarks: EPI Suite utilizes input values for relevant physicochemical parameters from its resident database, which has undergone extensive peer review and is accessed by input of the CAS number.
Reliability: (2) valid with restrictions
02-NOV-2001 (76)

Method: other (calculation): Fugacity Level III
Remark: Mass Distribution by Environmental Compartment

Air: 0.878%
Water: 23.3%
Soil: 52.4%
Sediment: 23.4%

Source: USEPA 2000.
Test substance: Benzene sulfonic acid, tridecyl- (25496-01-9); C13 was used in the EPI Suite modeling – the actual average range of alkyl chain lengths for dodecyl benzenesulfonic acid is 11.8-12.6
Remarks: EPI Suite utilizes input values for relevant physicochemical parameters from its resident database, which has undergone extensive peer review and is accessed by input of the CAS number.
Reliability: (2) valid with restrictions
02-NOV-2001 (76)

Method: other (calculation): Fugacity Level III
Remark: Mass Distribution by Environmental Compartment

Air: 1.14%
Water: 34.1%
Soil: 64.4%
Sediment: 0.367%

Source: USEPA 2000.
Test substance: Linear Alkylbenzene Sulfonate (LAS) (25155-30-0 et al.) (The modeled material was a C12-LAS)
Remarks: EPI Suite utilizes input values for relevant physicochemical parameters from its resident database, which has undergone extensive peer review and is accessed by input of the CAS number.
Reliability: (2) valid with restrictions
20-FEB-2003 (76)

3.4 Mode of Degradation in Actual Use

Memo: The LAB sulfonic acids are intermediates in the production of LAS.
11-OCT-2001

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge
Concentration: 11.3 mg/l related to DOC (Dissolved Organic Carbon)
Contact time: 28 day
Degradation: = 94 % after 28 day
Result: readily biodegradable
Method: other: OECD DOC-Die away test (EG - Richtlinie 92/69 EWG, Tiel II, C.4-A)
Year: 1992 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Source: Kurtin 1994.
Reliability: (1) valid without restriction
05-DEC-2001 (33)

Type: aerobic
Inoculum: domestic sewage
Concentration: 11.6 mg/l related to Test substance
Contact time: 37 day
Degradation: = 92 % after 37 day
Method: other: Modified coupled units test
Year: 1991 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Source: Kurtin 1994; Schoberl 1991.
Reliability: (1) valid without restriction
04-DEC-2001 (34) (67)

Type: aerobic
Inoculum: activated sludge
Concentration: 10 mg/l related to DOC (Dissolved Organic Carbon)
20 mg/l related to DOC (Dissolved Organic Carbon)
Contact time: 28 day
Degradation: = 69 % after 28 day
Method: OECD Guide-line 301 B "Ready Biodegradability: Modified Sturm Test (CO2 evolution)"
Year: 1992 **GLP:** no data
Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)
Remark: % degradation refers to mineralization.
Source: Stepan; OECD 1992.
Reliability: (2) valid with restrictions
03-JUL-2001 (61) (69)

Type: aerobic
Inoculum: activated sludge, domestic, non-adapted
Concentration: 10.8 mg/l related to DOC (Dissolved Organic Carbon)
Contact time: 28 day
Degradation: = 93 % after 28 day
Result: readily biodegradable
Kinetic: 7 day = 59 %
14 day = 73 %
21 day = 82 %
Method: other: Directive 79/831/EEC, Appendix V, C.4-A. DOC Die-Away Test
Year: 1990 **GLP:** yes
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Remark: The many biodegradation studies for LAS all report that LAS is readily biodegradable.
Source: Huels 1993.
Reliability: (2) valid with restrictions
11-OCT-2001 (21)

3.6 BOD5, COD or BOD5/COD Ratio

Remark: Not an HPV Challenge endpoint.
21-MAR-2003

3.7 Bioaccumulation

Species: Leuciscus idus melanotus (Fish, fresh water)
Exposure period: 3 day
Concentration:
BCF: = 130
Elimination:
Method: other: Golden ide were exposed to a constant water concentration of the dissolved test material for 3 days.
Year: **GLP:** no
Test substance: other TS: Dodecylbenzenesulphate sodium salt as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Remark: A BCF of 130 indicates a moderate affinity for uptake in fish tissues. However, uptake into tissues may be offset by metabolism and/or excretion.
Source: Freitag et al. 1985.
Reliability: (1) valid without restriction
11-OCT-2001 (14)

Species: Pimephales promelas (Fish, fresh water)
Exposure period: 48 hour(s)
Concentration: 2.7
BCF: = 22 - 87
Elimination: yes
Method: OECD Guide-line 305 E "Bioaccumulation: Flow-through Fish Test"
Year: 1981 **GLP:** yes
Test substance: other TS: LAS (C10-13), tested individually and as mixtures, activity: >97.4%
Method: The exposure phase in Experiment A was 48-hours. The exposure phase in Experiments B-D ranged from 168 to 192 hours. Fish were then transferred to untreated water for the depuration phase.
Remark: BCF values ranged between 2-1000 L/kg with BCFs increasing with increasing alkyl chain length. To address differences in composition of mixtures, bioconcentration potential was evaluated for a mixture typical of LAS in European detergent formulations (C10 12%, C11 29%, C12 34%, C13 24%; average alkyl chain length = C11.6) and a mixture typical of LAS in filtered Mississippi river water (C10 45%, C11 23%, C12 23%, C13 2%; average chain length = C10.8). The respective BCFs were 87 and 22 L/kg at concentrations of 2.7 and 4.1 uM, indicating that environmental processes decrease the bioconcentration potential of LAS.
Source: Tolls 1997; OECD 1981.
Test condition: The type of test was measured and flow-through.
Reliability: (2) valid with restrictions
20-FEB-2003 (51) (74)

3.8 Additional Remarks

Memo: None
02-NOV-2001

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:**
LC50: = 5.6
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1984 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5); 97.7% purity
Remark: The LC0 and LC100 were 4 and 8 mg/L, respectively. All water quality parameters were in compliance with OECD Guideline requirements. Ten fish (2-3 cm; 0.6 g/fish bw) were used per test concentration and control. Nominal test concentrations were 0.99, 2, 4, 8, and 16 mg/L. Dissolved oxygen saturation ranged from 84-90%, test temperature was 21.2-22.5 degrees C, and pH was 7.8-8.1. No affects were noted in the controls and no other affects were observed in the test concentrations.
Source: Kurtin 1997; OECD 1984.
Reliability: (1) valid without restriction
02-JUL-2001 (36) (58)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC0: = 4
LC50: = 4.1
LC100: = 4.3
Method: other: DIN 38412 Part 15
Year: **GLP:** yes
Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene sulfonic acid dodecyl- (27176-87-0)
Remarks: Standard test methodologies were employed following acceptable DIN Guidelines. Further details on test procedures were not provided by the authors.
Source: Knie et al. 1983
Reliability: (1) valid without restriction
03-JUL-2001 (7) (30)

Type: static
Species: Brachydanio rerio (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: = 10
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 **GLP:** yes
Test substance: other TS: Dodecylbenzenesulfonate-sodium salt as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Source: OECD 1992; IUCLID 1995.
Reliability: (2) valid with restrictions
Company GLP report cited in IUCLID Data Sheet but not available for review.
03-JUL-2001 (19) (60)

Type: other: daily renewal
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: = 4.3
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 **GLP:** no
Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)
Remark: LC50 is geometric mean of lower (3.2 mg/L) and upper (5.6 mg/L) limits from a series of studies investigating the reduction in number of individuals needed for testing. No further details on test parameters were provided but the study was conducted at Huntingdon Research Centre, which is a GLP testing laboratory.
Source: OECD 1992; Douglas et al. 1986.
Reliability: (1) valid without restriction
03-JUL-2001 (10) (60)

Type: static
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = 3
Method:
Year: 1981 **GLP:** yes
Test substance: other TS: Dobanic acid 102 (linear alkyl benzenesulfonic acid, C10-13) as a surrogate for Benzene sulfonic acid, tridecyl- (25496-01-9)
Method: Five aquaria were filled with a series of concentrations between 0.2 and 5 mg/l of Dobanic acid 102. Another aquarium served as a control. Five fingerling fish (mean weight 5.2 g) were placed in each aquarium. Test concentrations were 0.2, 0.5, 1, 2, and 3 mg/L. Standand physicochemical parameters were maintained pH 8.0±0.4, temperature 15±1 degree C, water hardness 230±10 mg/L as carbonate, and dissolved oxygen 9.9±0.3 ppm. All fish died at 5 mg/L by 96 hours, while no mortality was observed in any of the other concentrations. Graphical interpolation was used to determine the LC50 value.
Source: Stephenson 1981.
Reliability: (1) valid without restriction
03-JUL-2001 (70)

Type: semistatic
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: = 5.8
Method: OECD Guide-line 203 "Fish, Acute Toxicity Test"
Year: 1992 **GLP:** no data
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Remark: Analysis showed 92% of nominal concentration, tap water, water hardness; 96-120 mg/L CaCO3, pH 6.8-7.3, daily renewal, 14.5-16 C; life-stage: 5 months.
Source: Procter & Gamble 1991; OECD 1992.
Reliability: (1) valid without restriction
11-OCT-2001 (60) (63)

Type:
Species: Lepomis macrochirus (Fish, fresh water)
Exposure period:
Unit: mg/l **Analytical monitoring:**
LC50: = 3
Method:
Year: **GLP:**
Test substance: other TS: LAS normalized to C11.6
Remark: Mean LC50 for bluegill sunfish was derived from a total of 88 records compiled from several literature reviews.
Source: van de Plassche et al. 1999.
Reliability: (4) not assignable. This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary. However, because the original authors did in fact evaluate the data, and the study was published in a peer reviewed journal, the data are considered reliable.
21-FEB-2003 (77)

Type:
Species: Pimephales promelas (Fish, fresh water)
Exposure period:
Unit: mg/l **Analytical monitoring:**
LC50: = 3.2
Method:
Year: **GLP:**
Test substance: other TS: LAS normalized to C11.6
Remark: Mean LC50 for fathead minnow was derived from a total of 35 records compiled from several literature reviews.
Source: van de Plassche et al. 1999.
Reliability: (4) not assignable This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary. However, because the original authors did in fact evaluate the data, and the study was published in a peer reviewed journal, the data are considered reliable.
21-FEB-2003 (77)

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 5.2 (range 3.5-6.0)
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: other TS: 4-C10-13 Alkylbenzene sulfonic acid (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5); 97.7% purity
Remarks: Seven concentrations and a control were tested (0.4, 0.7, 1.2, 2.0, 3.5, 6.0, and 10 mg/L). Physicochemical parameters were maintained within acceptable ranges (temperature 20±1 degree C; dissolved oxygen 7.7-8.0; pH 7.8-8.0). At 48 hours, 0/20 daphnids were immobile in the 0.4 through 3.5 mg/L concentrations, 14/20 in 6.0 mg/L, and 20/20 in 10 mg/L. Graphical interpolation was used to calculate the EC50 value.

Source: Kurtin 1995; OECD 1984

Reliability: (1) valid without restriction
21-FEB-2003 (35) (62)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: = 9.3 - 11.6
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 **GLP:** yes
Test substance: other TS: See Remark
Remark: Daphnia less than 24 hours old were used. Test temperature was 20 degrees C, with twenty daphnids per concentration. Probit was used for the statistical analysis.
Remark: The toxicity values of the LAB sulfonic acids are in the same order as their sodium salts. As the chain length gets longer, the LC50 decreases. Three LAB sulfonic acids of varying chain lengths neutralized with caustic soda to obtain the sodium salt derivative were tested. Acid A had 48.4% of its weight in the C11 range and the majority its chain length ranged from C10-C13. Acid B had 49.4% of its weight in the C11 range and 31.7% of its weight in the C12 range. The majority of its chain length ranged from C10 to C12. Acid C had the majority of its chain length in the C10 to C13 range, almost evenly distributed between C11 and C12.
Result: Acid A had a LC50 of 11.6 mg/L, acid B 10.8 mg/L, and acid C 9.3 mg/L.
Source: Verge and Moreno 2000; OECD 1984.
Reliability: (1) valid without restriction
21-FEB-2003 (57) (79)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 2.9 (95% confidence limits 2.3-3.6 mg/L)
Method: Static tests were conducted. The test solution was added to dishes in concentrations of 0.3, 1, 2, 5, 10, and 20 mg/l with controls, in triplicate. Ten organisms (<24 hours old) were added to each dish. Immobilised organisms were recorded at 24 and 48 hours.
Year: 1981 **GLP:** yes
Test substance: other TS: Dobanic acid (linear alkyl benzenesulfonic acid, C10-13) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: Physicochemical parameters were maintained within acceptable ranges (temperature 20±1 degree C; pH 8.2±0.1; hardness 240±10 mg/L as carbonate; dissolved oxygen 10.2±0.2 ppm). Probit analysis was used to determine the EC50. At 48 hours, the number of daphnids immobilized/number in concentration were 0/30, 3/30, 8/30, and 22/30 at 0.3, 1, 2, and 5 mg/L. All daphnids were immobilized at both 10 and 20 mg/L at 48 hours.
Source: Stephenson 1981.
Reliability: (1) valid without restriction
21-FEB-2003 (70)

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC0: = 6
EC50: = 12
EC100: = 14
Method: other: DIN 38412 Part 11. All parameters were maintained in accordance with acceptable DIN guidelines. No further details on methods were provided.
Year: **GLP:** yes
Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Source: Knie et al. 1983.
Reliability: (1) valid without restriction
20-FEB-2003 (6) (30)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 5.88
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: **GLP:** no data
Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)
Source: Galassi et al. 1992; EEC Directive.
Reliability: (2) valid with restrictions
Data as cited in IUCLID data sheet.
20-FEB-2003 (9) (15)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: = 4.3 (95% confidence limits 3.5-4.7 mg/L)
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test".
Year: 1984 **GLP:** yes
Test substance: The substance tested was derived from a LAB product with 67.0% of its weight in the C13 range. The rest of the weight is spread over the C10-C14 range. Used as a surrogate for benzene sulfonic acid, tridecyl- (25496-01-9).
Remarks: Twenty daphnids (<24 hours old) were place in each concentration and maintained at 20 degrees C. Probit analysis was used to determine the EC50.
Source: Verge and Moreno. 2000; OECD 1984.
Reliability: (1) valid without restriction
21-FEB-2003 (57) (79)

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 6.8
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: 1984 **GLP:** yes
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Source: EEC Directive 1984.
Reliability: (1) valid without restriction
21-FEB-2003 (9)

Species: Daphnia magna (Crustacea)
Unit: mg/l
EC50: = 4.1
Test substance: other TS: C10-13 LAS (CAS #68411-30-3)
Remark: D. magna was selected as the representative test organism of the toxicity of LAS to invertebrates. The value is a mean of 17 records of commercially representative LAS with C10-13 alkyl chain lengths and average carbon numbers of C11.6 and C11.8.
Source: HERA 2002.
Reliability: (4) not assignable This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary. However, because the original authors did in fact evaluate the data, and the study was published in a peer reviewed journal, the data are considered reliable.
21-FEB-2003 (18)

Species: Daphnia magna (Crustacea)
Unit: mg/l
EC50: = 4.7
Test substance: other TS: LAS normalized to C11.6
Remark: EC50 is geometric mean of 139 records compiled from literature reviews. Values range from 0.26 to 55 mg/L. This large range is caused by differences in the LAS tested with respect to alkyl chain and/or phenyl isomer distribution and differences in test design.
Source: van de Plassche et al. 1999.
Reliability: (4) not assignable This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary. However, because the original authors did in fact evaluate the data, and the study was published in a peer reviewed journal, the data are considered reliable.
21-FEB-2003 (77)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 36
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: The reported EC50 is for growth rate. The 72-hr EC50 for biomass was also tested in this experiment and determined to be 14 mg/L for this substance.
Source: Kurtin 1994; OECD 1984.
Reliability: (1) valid without restriction
21-FEB-2003 (32) (56)

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 4 day
Unit: mg/l **Analytical monitoring:** no
EC50: = 170 (95% confidence interval 140-230 mg/L)
Method: other: Twelve flasks were filled with quantities of test solution of 2, 3, 4.6, 7, 11, 16, 25, 38, 57, 87, 130, and 200 mg/L. Six flasks served as controls. Algae was added to each container at an initial concentration of 5 x 10^3 cells/mL. Flasks were incubated in a cooled, orbital incubator (100 cycles/min) under constant illumination at 24±1 degree C. Cell counts were made with a Coulter counter after 2 and 4 days. Probit analysis was used to determine the EC50.
Year: 1981 **GLP:** yes
Test substance: other TS: Dobanic acid (linear alkyl benzenesulfonic acid, C10-13) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Source: Stephenson 1981.
Reliability: (1) valid without restriction
21-FEB-2003 (70)

Species: Haematococcus pluvialis (Algae)
Endpoint: other: inhibition of oxygen production
Exposure period: 4 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50: = 50
Method: other: Based on the procedure by Tumpling. The initial cell density was 80,000 cells/mL. Standard protocols were followed.
Year: **GLP:** yes
Test substance: other TS: n-dodecylbenzenesulfonate as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Source: Knie et al. 1983.
Reliability: (1) valid without restriction
20-FEB-2003 (30)

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
EC50: = 29
Method: other: EPA method
Year: 1985 **GLP:** no
Test substance: other TS: Benzene sulfonic acid, dodecyl- (27176-87-0)
Source: Galassi et al. 1992; EPA 1985.
Reliability: (2) valid with restrictions
Data as cited in IUCLID data sheet.
20-FEB-2003 (15) (75)

Species: Scenedesmus subspicatus (Algae)
Endpoint: growth rate
Exposure period: 72 hour(s)
Unit: mg/l **Analytical monitoring:** no
EC50(C_{11}): = 240
EC50($C_{11.6}$): = 163
EC50(C_{13}): = 54
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test", with the test media recommended by AFNOR. Initial cell concentrations were 1. x 10^4 cells/mL. Algae was enumerated with a Coulter Counter.
Year: 1984 **GLP:** no data
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.); Molecular weights were 334, 343, and 363 for alkyl chain lengths C_{11}, $C_{11.6}$, and C_{13}, respectively.
Remarks: Toxicity increases as the average alkyl chain length increases, until it becomes almost insoluble, at which time toxicity decreases.
Source: Verge and Moreno 1996; OECD 1984.
Reliability: (2) valid with restrictions
21-FEB-2003 (56) (78)

Species: Various species
Unit: mg/l
IC50 : = 9.1
Test substance: other TS: C10-13 LAS (CAS #68411-30-30)
Remark: Data are for various algae species. The value is a geometric mean of 12 records of commercially representative LAS with C10-13 alkyl chain lengths and average carbon number of C11.6 and C11.8.
Source: HERA 2002.
Reliability: (4) not assignable This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary. However, because the original authors did in fact evaluate the data, and the study was published in a peer reviewed journal, the data are considered reliable.
21-FEB-2003 (18)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type:
Species:
Exposure period:
Unit: **Analytical monitoring:**
Method:
Year: **GLP:**
Test substance:
Remark: Not an HPV Challenge endpoint.
21-MAR-2003

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other: Brachydanio rerio, Pimephales promelas, Poecilia reticulata, Oncorhynchus mykiss, and Tilapia mossambica
Endpoint: other: growth
Exposure period: 28 day
Unit: mg/l **Analytical monitoring:** no
NOEC: = .25 - 3.2
Method:
Year: **GLP:** no data
Test substance: other TS: Linear Alkylbenzene Sulfonate (LAS) (68411-30-3 et al.)
Remark: All data were from tests conducted on commercial LAS with C10-13 alkyl chains and average carbon lengths of C11.6 and C11.8. The NOEC values have been normalized using QSARs to the average structure of C11.6 LAS.
Result: The article compiles the no observed effect concentration (NOEC) values for many tests conducted on an assortment of species. The following table shows the geometric mean NOEC values for each fish species (n = number of studies included for each species).

Species	Geometric mean NOEC (mg/L)	n
Brachydanio rerio	2.3	1
Pimephales promelas	0.87	14
Poecilia reticulata	3.2	1
Oncorhynchus mykiss	0.34	7
Tilapia mossambica	0.25	1

Source: van de Plassche et al. 1999.
Reliability: (4) not assignable This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary. However, because the original authors did in fact evaluate the data, and the study was published in a peer reviewed journal, the data are considered reliable.
21-MAR-2003 (77)

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Unit: mg/l
NOEC: = 1.4
Test substance: other TS: LAS normalized to C11.6
Remark: NOEC is geometric mean of 12 records compiled from literature reviews and normalized to C11.6.
Source: van de Plassche et al. 1999.
Reliability: (4) not assignable This study was given a reliability score of 4 because the original reports reviewed by the authors were not directly reviewed in the compilation of this robust summary. However, because the original authors did in fact evaluate the data, and the study was published in a peer reviewed journal, the data are considered reliable.
21-FEB-2003 (77)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:
Species:
Endpoint:
Exposure period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: Not an HPV Challenge endpoint.
20-FEB-20
03

4.6.2 Toxicity to Terrestrial Plants

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species

Species:
Endpoint:
Expos. period:
Unit:
Method:
Year: **GLP:**
Test substance:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

4.7 Biological Effects Monitoring

Memo: Not an HPV Challenge endpoint.
20-FEB-2003

4.8 Biotransformation and Kinetics

Type:
Remark: Not an HPV Challenge endpoint.
20-FEB-2003

4.9 Additional Remarks

Memo: None
11-OCT-2001

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: other: rat, Wistar
Sex: male/female
Number of Animals: 10
Vehicle: other: none
Value: = 1470 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1981 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: Five of each sex per dose level were tested. Test duration was 14 days. The dose range was 1250-1990 mg/kg.
Source: Murmann 1984; OECD 1981.
Reliability: (1) valid without restriction
21-FEB-2003 (46) (52)

Type: LD50
Species: other: rat, Sprague-Dawley CD
Sex: male/female
Number of Animals: 9
Vehicle: other: distilled water
Value: = 775 mg/kg bw
Method: other: Safepharm Standard Test Method Number 513.01
Year: 1998 **GLP:** yes
Test substance: other TS: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5); no activity % provided
Method: A group of three fasted males and three fasted females were treated with the starting dose (2000 mg/kg bw). As the females dosed with 2000 mg/kg bw died, a further three fasted males and three fasted females were treated with the dose level 300 mg/kg bw. The test material was administered orally as a solution in distilled water. The animals were observed 1/2, 1, 2, and 4 hours after dosing and then once daily for up to 14 days. Bodyweights were recorded on Day 0 (day of dosing) and on Days 7 and 14 or at death. At the end of the observation period the surviving animals were killed by cervical dislocation and all animals were subject to gross necropsy.
Remark: LD50 value is geometric mean between 300 and 2000 mg/kg bw. Three females were found dead one day after dosing at the 2000 mg/kg bw dose level. There were no deaths at the 300 mg/kg bw dose level. No clinical signs of toxicity were noted in animals treated with 300 mg/kg bw. The surviving animals showed expected gains in body weight over the study period. Abnormalities noted at necropsy of animals that died during the study were abnormally red lungs, dark liver, and dark kidneys.
Source: Hempstock 1998.

Reliability: (1) valid without restriction
21-FEB-2003 (17)

Type: LD50
Species: other: rat, Wistar
Sex: male/female
Number of Animals:
Vehicle: no data
Value: = 500 - 2000 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1987 **GLP:** yes
Test substance: other TS: Dodecylbenzenesulfonate, sodium salt as a surrogate for benzene sulfonic acid, dodecyl- (27176-87-0)
Source: OECD 1987; IUCLID 1995.
Reliability: (2) valid with restrictions
Company reported GLP study listed in IUCLID Data Set but not available for review.
02-JUL-2001 (20) (59)

Type: LD50
Species: rat
Sex: male/female
Number of Animals: 10
Vehicle:
Value: = 1080 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: 1981 **GLP:** no
Test substance: other TS: Marlon A 386 (CAS #68411-30-3) C10-13 LAS, average alkyl chain length = C11.6; Activity: 86%
Method: Five male and five female rats were given LAS doses of 1075, 1220, 1360, 1710 or a control by gavage. Body weight and other signs were measured on days 7 and 14. Temperature was maintained at 20+/-1°C with a 12 hr light-dark cycle. Animals were observed for 14 days after dosing.
Remark: Symptoms beginning about 30 minutes past application included diarrhea, squatting attitude, breathing difficulties, nose bleeding, ataxia, and lethargy. These symptoms had disappeared in surviving animals by 120 hours. Virtually all animals died in doses of 1220 mg/kg and above. Note that all doses are corrected for 86% activity. The original doses were 1250, 1415, 1580 and 1990 mg/kg.
Source: Murmann 1984a.
Reliability: (2) valid with restrictions
21-FEB-2003 (49)

Type: LD50
Species: other: Rat, CFY (Sprague-Dawley origin)
Sex: male/female
Number of Animals: 10
Vehicle:
Value: = 1980 mg/kg bw
Method: OECD Guide-line 401 "Acute Oral Toxicity"
Year: **GLP:** yes
Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na).
Method: Five male and five female rats were given single doses by gavage at 1500, 2350 and 3760 mg/kg bw. Rats were housed in cages grouped by sex and given standard laboratory diet and water ad libitum. Mean daily temperature was maintained at 21-22°C at a mean relative humidity of 56%. Lighting was on a 12 hrs dark and 12 hrs light photoperiod. Animals were observed for 14 days after dosing.
Remark: Four rats from each of the two lowest concentrations and all rats from the highest concentration died. All deaths occurred between 6 and 23 hours after dosing. Signs of reaction to treatment included pilo-erection, hunched posture, abnormal gait (waddling), lethargy, decreased respiratory rate, ptosis, pallor of the extremities, and diarrhea. All surviving animals appeared to recover completely by day 4. Autopsy of rats that died revealed isolated cases of pallor of the kidneys or spleen. Terminal necropsy findings for survivors were normal. Note that all doses are corrected for 47% activity. The original doses were 3200, 5000, and 8000 mg/kg.
Source: Kynoch 1986a.
Test substance: Activity 47%. Average alkyl chain length = C11.2 Clear yellow liquid.
Reliability: (1) valid without restriction
21-FEB-2003 (37)

5.1.2 Acute Inhalation Toxicity

Type: other: Approximate Lethal Concentration (ALC)
Species: other: Rat Crl: CD (SD) BR
Sex: male
Number of Animals: 6
Vehicle:
Exposure time: 4 hour(s)
Value:
Method: other
Year: 1992 **GLP:** no data
Test substance: other TS: LAS (CAS #25155-30-0); activity 98%
Method: Groups of six male 8-week old rats were restrained in perforated, stainless steel cylinders with conical nose pieces. Exposure was nose-only to an aerosol atmosphere for 4 hours. After exposure, rats were returned to their cages and observed for clinical signs for 14 days. Mean measured

concentrations in the test chambers were 65, 120, 260, and 310 mg/m3. Chamber temperature ranged between 25-26°C.

Remark: The ALC is defined as the lowest atmospheric concentration generated that caused death in 1 or more rats either on the day of exposure or within 14 days post exposure. No mortality occurred at concentrations up to 260 mg/m3. At 310 mg/m3, one rat died during exposure and 2 rats died one day post exposure. The test material is considered moderately toxic by inhalation. However, it is important to note that this laboratory exposure is not representative of the possible LAS exposure during actual use. In this study, animals were given high exposures to respirable-sized particles. Spray products containing LAS are designed to produce large particle sizes. These large particles are needed for efficient delivery of the spray to the surface being cleaned. This results in particle sizes that are much larger than the respirable particle sizes used in testing and therefore would not be able to reach far into the lungs where effects could occur. Given this lack of relevance to real-world exposure potential, the use of this study for risk assessment purposes is limited.

Result: 310 mg/m3 of particulate

Source: Kinney 1985.

Reliability: (2) valid with restrictions

21-FEB-2003 (29)

5.1.3 Acute Dermal Toxicity

Type: LD50

Species: rabbit

Sex:

Number of Animals: 6

Vehicle:

Value: = 2000 mg/kg bw

Method: other: Test material was applied to shaved area of back of 6 rabbits at two doses: 2000 mg/kg (undiluted) and 212 mg/kg (2% aqueous dilution). The areas were covered with plastic and left in contact with test material for 24 hours.

Year: **GLP:** no

Test substance: other TS: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)

Remark: All of the animals exposed to the 212 mg/kg survived. Mortality occurred in three out of six rabbits exposed to the undiluted dose. No untoward behavioral reactions were observed. Necropsy did not reveal any gross pathological alterations. Local skin reactions included erythema, mild edema and mild desquamation at 212 mg/kg and chemical burns, severe edema and necrosis at 2000 mg/kg.

Result: LD50 = 2000 mg/kg bw (undiluted); LD50 > 212 mg/kg bw (2% aqueous dilution)

Source: Kretchmar 1972.

Reliability: (1) valid without restriction

21-FEB-2003 (31)

Type: LD50
Species: other: Rat, CFY (Sprague-Dawley origin)
Sex: male/female
Number of Animals: 10
Vehicle:
Value: > 2000 mg/kg bw
Method: OECD Guide-line 402 "Acute dermal Toxicity"
Year: **GLP:** yes
Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). activity 47%. Average alkyl chain length = C11.2. Yellow, viscous liquid.
Method: Five male and five female rats were exposed to 2000 mg/kg in a limit test. The test substance was applied to clipped intact skin in the dorso-lumbar region and covered with gauze held in place with an impermeable dressing. The dressing was removed after 24 hours and the treated area of the skin washed with warm water and blotted dry. Observations for dermal irritation were made daily for 14 days.
Remark: There were no deaths or signs of a systemic reaction following a single dermal application at 2000 mg/kg bw. Well defined or slight erythema and slight oedema were observed at all test sites after removal of the occlusive dressing on Day 2. All test sites were entirely covered by scab formation from Day 7. Sloughing from the scabbed skin began at various times between Day 7 and Day 12 and was completed before termination. Low bodyweight gains or loss of body weight were recorded for one male and three females in Day 8. Two of the same females and a third female also showed low bodyweight gain between Days 8 and 15.
Source: Kynoch 1986b.
Reliability: (1) valid without restriction
21-FEB-2003 (38)

5.1.4 Acute Toxicity, other Routes

Type:
Species:
Sex:
Number of Animals:
Vehicle:
Route of admin.:
Value:
Method:
Year: **GLP:**
Test substance:
Remark: Not a required OECD or HPV endpoint.
08-FEB-2001

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration: .5 other: mL

Exposure:
Exposure Time: 4 hour(s)
Number of Animals: 6
PDII:
Result: highly irritating
EC classificat.: irritating
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1981 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: The shaved treated area was covered for the first 4 hours. Observations were made after 1, 24, 48, 72 hours and 6, 9, and 14 days. The irritation index was 5.25.
Source: Murman 1984; OECD 1981.
Reliability: (1) valid without restriction
20-FEB-2003 (48) (53)

Species: rabbit
Concentration: .5 other: mL

Exposure:
Exposure Time: 4 hour(s)
Number of Animals: 6
PDII:
Result: corrosive
EC classificat.: irritating
Method: Draize Test
Year: 1965 **GLP:**
Test substance: other TS: Benzene sulfonic acid dodecyl- (27176-87-0)
Method: The test material was applied as submitted to the intact skin and covered with a "1 x 1" gauze patch held in place with saran wrap. At the end of 4 hours, the coverings were removed and the area examined for skin irritation and corrosion. Examinations were repeated at 24 and 48 hours and scored according to Draize 1965.
Remark: The primary dermal irritation scores were 3.4, 6.3, and 7.0 at 4, 24, and 48 hours, respectively.
Source: Thompson 1980.
Reliability: (1) valid without restriction
02-NOV-2001 (1) (11) (71)

Species: other: New Zealand albino rabbits
Concentration: .5 other: mL

Exposure:
Exposure Time: 4 hour(s)
Number of Animals: 6
PDII:
Result: moderately irritating
EC classificat.:
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: **GLP:** yes
Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). Activity 47%. Average alkyl chain length = C11.2. Clear yellow liquid.
Method: A 0.5 ml aliquot of P-500 N-Na was applied under a 2.5 cm2 gauze pad to an approximate 10 cm2 area of clipped intact skin of 3 rabbits. Each treatment site was occluded with an elastic adhesive dressing for four hours, after which the dressing was removed and the area washed with distilled water. Examination of the treated skin was made approximately 30 minutes after removal of the patch and daily through 14 days. Grading and scoring of the dermal reactions was performed using the standard numerical scoring system.
Remark: Well defined to moderate skin reactions were observed in all three animals following removal of the bandages. Desquamation of the stratum corneum was observed in all three animals. The reaction in all three animals gradually ameliorated from Days 5, 10 and 11, respectively, and had all resolved completely in one animal by Day 12.
Source: Liggett and Parcell 1986a.
Reliability: (1) valid without restriction
21-FEB-2003 (41)

5.2.2 Eye Irritation

Species: rabbit
Concentration: .1 other: mL
Dose:
Exposure Time: 144 hour(s)
Comment:
Number of Animals: 6
Result: moderately irritating
EC classificat.: irritating
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1981 **GLP:** no
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: Treatment was to the right eye with lower lid removed. The left eye was untreated. The eyes were not washed out during the test. Observations were made at 1, 24, 48, and 72 hours

and at 6 days after application. The total irritation index was 46.9.

Source: Murmann 1984; OECD 1981.

Reliability: (1) valid without restriction

20-FEB-2003 (47) (54)

Species: other: New Zealand albino rabbits

Concentration: .1 other: mL

Dose:

Exposure Time:

Comment:

Number of Animals: 9

Result: irritating

EC classificat.:

Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"

Year: 1981 **GLP:** yes

Test substance: other TS: Alkylbenzene sulfonate, sodium salt (designated as P-500 N-Na). Activity 47%. Average alkyl chain length = C11.2. Clear yellow liquid.

Method: Nine rabbits received a 0.1 mL aliquot of P-500 N-Na placed into the lower everted lid of one eye per animal. For three rabbits the eyelids were then gently held together for one second before releasing. For three other rabbits the eyes were irrigated with water for 5 minutes following a 4-second exposure. For the remaining three rabbits the eyes were irrigated for 5 minutes following a 30-second exposure. Eyes were examined after 1 hour and 1, 2, 3, 4, 7, 14 and 21 days after exposure. Grading was performed using the standard scoring system.

Remark: The following results were noted:

1) Three animals without any rinsing: averaged irritation scores (24, 48, 72 hours) for each animal: cornea 2.3, 1.7, 2; iris: 1.3, 0, 0; conjunctivae redness: 3, 1.7, 2; conjunctivae chemosis: 3, 2, 2. In the first animal the effects were persistent at day 14.

2) Three animals with rinsing for five minutes following a 30 second exposure: averaged scores: cornea 0.7, 1, 1.3; iris: 0, 0.7, 0.3; conjunctivae redness: 1.7, 2, 1.3; conjunctivae chemosis: 2, 1.3, 2. The eyes were normal 7 or 14 days after instillation.

3) Three animals with rinsing for five minutes following a 4 second exposure: averaged scores: cornea 0.7, 2.3, 0.7; iris: 0, 0, 0; conjunctivae redness: 1.7, 1.7, 1; conjunctivae chemosis: 1.3, 2, 1. The eyes were normal 7 days after instillation.

Findings lead to a definition of irritating for LAS at 47% applied without rinsing, irritating (even if with lower effects, mainly as cornea opacity and conjunctivae redness) with rinsing after 30 second of exposure, and not irritating

with rinsing after 4 second of exposure.
Overall, instillation of P-500 N-Na into the eyes of rabbits elicited positive responses in all animals. Irrigation of the eyes only slightly reduced the irritation potential.
Source: Liggett and Parcell 1986b.
Reliability: (1) valid without restriction
21-FEB-2003 (42)

5.3 Sensitization

Type: other: sensitization
Species: guinea pig
Number of Animals: 20
Vehicle: other: corn oil
Result: not sensitizing
Classification:
Method: other: Magnusson and Kligman
Year: 1969 **GLP:** yes
Test substance: other TS: Dobanic acid 103 (Benzenesulfonic acid, C10-13) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: In a guinea-pig maximization test none of the test animals showed positive responses at 24 or 48 hours after removal of the challenge patches. The test material showed no sensitizing potential in guinea pigs.
Source: Rose 1983.
Reliability: (1) valid without restriction
21-JAN-2002 (44) (66)

Type: Guinea pig maximization test
Species: other: guinea pig, Hartley
Number of Animals: 20
Vehicle: water
Result: not sensitizing
Classification: not sensitizing
Method: other: OECD Guideline 406; Directive 179/831 Annex, Part B.
Year: 1981 **GLP:** yes
Test substance: other TS: LAS, activity: 50%; average alkyl chain length = C11.6
Remark: Solutions of LAS were applied intracutaneously and epicutaneously to 10 male and 10 female animals. Induction concentration was 25% in water; the challenge concentration was 12.5%. No positive responses were observed.
Source: RBM 1985.
Reliability: (1) valid without restriction
21-FEB-2003 (64)

Type: other: sensitization
Species: guinea pig
Number of Animals: 10
Vehicle: deionized water
Result: see remarks
Classification: see remarks
Method: other: Magnusson-Kligman Maximization Test
Year: 1992 **GLP:** yes
Test substance: A mixture containing 68.4% water, 17.5% dodecylbenzene sulfonic Acid (CAS #27176-87-0), 11.76% polymethacrylate (CAS #25087-26-7), 2.3% sodium hydroxide (CAS #1310-73-2), and 0.040% unknowns
Remark: There was some evidence of slight erythema at the undiluted dose, but nothing at 75% or below. Moderate to intense erythema was evident in all animals following the first challenge dose. During the second challenge, 3 of 8 animals did not elicit sensitization responses while 2 of 8 had possible sensitization reactions. Another 3 of 8 could not be assessed due to the level of irritation seen in both the test and naive animals. Interpretation of this study is difficult since it is unclear which component of the mixture may have caused the reactions observed. Based on the fact that no sensitization was observed in other studies conducted on LAS and LAB sulfonic acids, the Coalition believes the sensitization is likely the result of exposure to the other compounds present in the mixture.
Source: Glaza 1992.
Reliability: (4) not assignable. Because of the questions regarding which component of the mixture may have contributed to the effects observed, this study cannot be used in the assessment of LAB sulfonic acids.
30-JAN-2004 (15)

5.4 Repeated Dose Toxicity

Species: rat **Sex:** male/female
Strain: Wistar
Route of admin.: drinking water
Exposure period: 9 months
Frequency of treatment: Daily in drinking water
Post. obs. period:
Doses: 0.07, 0.2%, 0.6% (85, 145, 430 mg/kg bw d)
Control Group: yes
NOAEL: 0.07% (85 mg/kg bw d)
LOAEL: 0.2% (145 mg/kg bw d)
Method: Groups of 8-9 male and 8-9 female rats were given LAS for 9 months.
Year: **GLP:** no
Test substance: other TS: C10-14 LAS (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = C11.7

Remark: Information as cited in IPCS document. This study represents the most appropriate NOAEL value accepted by OECD at SIAM 17. The LAS Coalition reviewed fifteen studies in which rodents (rats and mice) and non-rodents (monkeys) received repeated exposures to LAS via the oral or dermal routes. Test durations ranged from 15 days up to 9 months in those studies. LOAELs ranged from 115 to 750 mg/kg bwd and the highest NOAEL (below the lowest LOAEL) was found to be the 85 mg/kg bwd resulting from the study summarized here.

Result: Body weight gain was suppressed in the male 0.6% group. Haematological, serum-biochemical, and enzymatic parameters of the liver and kidney were also affected in the high dose groups. No organ weight changes were observed. The intake of LAS was 50 mg/kg bw d in the male 0.07% group. The values for the 0.2% group were 120 and 170 mg/kg bw d for males and females, respectively.

Source: European Commission 2000a; Yoneyama et al. 1976.

Reliability: (4) not assignable. This study was assigned a reliability score of 4 because the original report was not available for review. However, the study was evaluated by IPCS prior to inclusion in their criteria document; therefore it is considered to be reliable.

21-MAR-2003 (12) (81)

5.5 Genetic Toxicity 'in Vitro'

Type: other: Bacterial reverse mutation assay (Ames test)
System of testing: Salmonella typhimurium TA 98 and TA 100
Concentration: 1.5 to 1500 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: Ames
Year: **GLP:** yes
Test substance: other TS: Benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: The test material was tested up to its toxic limit.
Result: No significant increases in the frequency of revertant colonies were recorded for either of the bacterial strains with any dose of the test substance, either with or without metabolic activation.
Source: Thompson 1998.
Reliability: (1) valid without restriction
05-NOV-2001 (72)

Type: Ames test
System of testing: Salmonella typhimurium TA 1535, TA 1537, TA 1538, TA 98, TA 100
Concentration: 8, 40, 200, 1000 and 5000 ug/plate; 3 replicates per concentration
Metabolic activation: with and without S9 metabolic activation
Result: negative
Method: Directive 84/449/EEC, B.14 "Other effects - Mutagenicity (Salmonella typhimurium - reverse mutation assay)"
Year: 1984 **GLP:** yes
Test substance: other TS: Marlon A 390 (CAS #68411-30-3) C10-13 LAS, average alkyl chain length = C11.6; activity 91.3%
Remark: Negative (water) and positive (sodium azide, aminoacridine, and nitrofluorene) controls were used.
Result: Cytotoxicity concentration:
With metabolic activation: > 5000 ug/plate
Without metabolic activation: > 5000 ug/plate
Source: EEC Directive 1984; Schoeberl 1993a.
Reliability: (1) valid without restriction
21-FEB-2003 (8) (68)

Type: other: transformation test with SHE-cells
System of testing: Syrian hamster embryo (SHE) cells
Concentration: up to 50 ug/ml
Metabolic activation: without
Result: negative
Method:
Year: **GLP:** no
Test substance: other TS: C10-14 LAS, sodium salts (CAS #69669-44-9)
Method: Cell cultures were prepared and plated in 75 cm2 flasks containing 20 mL of culture medium. On day 5, target cells were trypsinized and a suspension of target cells was added to the solution plated on complete medium. Plates were dosed on day 6. Nine dishes were used for each dose level. On day 14, the cultures were fixed, stained, and examined to count normal and transformed colonies.
Remark: LAS did not produce transformation at any of the doses tested.
Source: Inoue et al. 1980.
Test substance: average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = C11.7; activity: 22.2%
Reliability: (2) valid with restrictions
21-FEB-2003 (26)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse **Sex:** male/female
Strain: NMRI
Route of admin.: other: oral intubation
Exposure period: 72 hours
Doses: 1122 mg/kg bw
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: 1983 **GLP:** yes
Test substance: other TS: Benzenesulfonic acid, C10-13-alkyl derivatives (85536-14-7; 97.3% purity) as a surrogate for benzene sulfonic acid, C10-16-alkyl derivatives (68584-22-5)
Remark: Forty male and forty female mice were exposed to 1122 mg/kg bw. The positive control was cyclophosphamid and the negative control was the vehicle, 0.9% NaCl. No significant increases in the number of polychromatic erythrocytes with micronuclei were observed.
Source: Fedtke 1991; OECD 1983.
Reliability: (1) valid without restriction
11-OCT-2001 (13) (55)

Type: other: Mammalian bone marrow cytogenetic assay
Species: other: mouse: ICR: JCL **Sex:** male
Strain: ICR
Route of admin.: gavage
Exposure period: 5 days and 1 day
Doses: 200, 400, 800 mg/kg
Result: negative
Method: other: Chromosomal aberrations were examined 6, 24, 48 hours after administration.
Year: **GLP:** no
Test substance: other TS: C10-14 LAS, sodium salt (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2000) = 11.7
Remark: Besides the pure LAS, commercial preparation containing 19% LAS and another containing 17.1% LAS were given to mice as single doses only by gavage at 800, 1600 or 3200 mg/kg bw d and 1000, 2000 or 4000 mg/kg bw d, respectively. The highest doses were 50% of the respective LD50 values. No significant differences in the incidence of chromosomal aberrations were observed in any LAS treatment relative to the controls. Information as cited in the IPCS document.
Result: There was no significant difference in the incidence of chromosomal aberrations between any of the groups given LAS and the negative control group.
Source: Inoue et al. 1977; European Commission 2000a.
Reliability: (4) not assignable
20-FEB-2003 (12) (25)

5.7 Carcinogenicity

Species: rat **Sex:** male/female
Strain: other: Charles River
Route of admin.: oral feed
Exposure period: 2 years
Frequency of treatment: continuous in feed
Post. obs. period:
Doses: 0.02, 0.1, 0.5% (10, 50, 250 mg/kg bw d
Result:
Control Group: other: yes, concurrent no treatment, positive, and historical controls
Method:
Year: **GLP:** no
Test substance: other TS: C10-14 LAS, sodium salt (CAS# 69669-44-9); 98.1% activity on an anhydrous basis (41.9% active)
Method: Four groups of Charles River weanling rats, divided by sex, were given 0.5, 0.1, and 0.02% LAS in their food for 2 years. Following completion of those studies, five male and five female rats from each of the parental groups (F1b and F2b) and all survivors were selected for necropsy. Body weight and organ to body weight ratios were recorded, and routine hematology and histology were performed. Weanling animals for

the F3a generation were similarly treated. Mytomycin C was used as a positive control at a dose of 5 mg/kg and induced severe chromosomal aberrations.

Result: Gross examination of all animals for pathology did not reveal any abnormalities. No consistent dietary induced changes that could be considered a toxic response were observed. Animals that showed significant loss of weight, development of tumors, or other evidence of abnormalities were sacrificed and tissues examined. The incidence of tumors and the common incidental diseases were similar in all dieting groups.

Source: Buehler et al. 1971.

Reliability: (2) valid with restrictions

27-MAR-2003 (2)

5.8 Toxicity to Reproduction

Type: other: 3-generation reproduction study
Species: rat **Sex:** male/female
Strain: other: Charles River
Route of admin.: oral feed
Exposure Period: 2 years
Frequency of treatment: continuous in feed
Premating Exposure Period
male: 84 days
female: 84 days
Duration of test: 3 generations
Doses: 0.02, 0.1, 0.5% (14, 70, 350 mg/kg bw d)
Control Group: yes
NOAEL Parental: = 350 mg/kg bw
NOAEL F1 Offspr.: = 350 mg/kg bw
NOAEL F2 Offspr.: = 350 mg/kg bw
Year: 1971 **GLP:** no
Test substance: other TS: Sodium salt LAS (C10-14), activity: 98.1% on an anhydrous basis (41.9% active)

Method: Na-LAS (chain length distribution C10-14) was fed for 84 days to 4 groups of weanling rats (3 dose levels, plus control), each dose consisting of 50 animals each of both sexes (PO-generation). When the P0 generation was 107-112 days old, 20 females from each dose group were mated with 20 males from the same group and maintained together for 17 days. The first litters of each generation (Fla- and F2a-generation) were sacrificed at 21 days of age. Ten days after the final litter was sacrificed, all females were remated with different males from the same group to obtain the F1b generation. From the Flb-generation, 20 males and females of each group were selected at weaning to continue their respective diets and to be used for further reproduction studies. Reproduction studies on the F1b and F2b generations were started when the rats were 80 to 85 days old, and were continued until the F3b generation was weaned.

Result: Results were reported as no effects at the highest

concentration tested (0.5% in the diet). General reproduction including fertility gestation, parturition, neonatal viability, lactation, and post-weaning growth was normal for all test groups and did not deviate from the controls in each generation. No gross abnormalities were noted. No definitive adverse effects due to the test material were noted in the haematology and pathology.

Remarks: A total of three reproductive toxicity studies were reported for LAS and no reproductive or fertility effects were observed in any of the studies. NOAELs ranged from 70 to 350 mg/kg bw d, which were the highest doses tested.

Source: Buehler et al. 1971.

Reliability: (2) valid with restrictions

20-FEB-2003 (2)

5.9 Developmental Toxicity/Teratogenicity

Species: rat **Sex:** female
Strain: other: SD-JCL
Route of admin.: oral feed
Exposure period: from day 0 to 20 of gestation
Frequency of treatment: daily **GLP:** no
Doses: 0.1%, 1.0% (80, 780 mg/kg bw d)
Control Group: yes
NOAEL Maternalt.: = 780 mg/kg bw
NOAEL Teratogen.: = 780 mg/kg bw
Method: other: LAS was fed in the diet to 16 pregnant female rats/dose from day 0 to 20 of gestation.
Test substance: other TS: Japan LAS; average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = C11.7-12.3.
Remark: Information as cited in IUCLID Data Sheet and IPCS document. This study represents the most appropriate NOAEL value identified by the Industry Coalition for the SIDS Assessment of LAS. The LAS Coalition reviewed ten developmental toxicity studies conducted on rats, mice and rabbits in which the test animals received LAS via the oral route (feed, gavage, or drinking water). While effects were observed at maternally toxic doses, no decreases in litter size, no changes in litter parameters, and no malformations or significant differences in skeletal defects were observed in these studies at oral doses up to 780 mg/kg bwd. Note also that the NOAEL used in the risk assessment is derived from the repeated dose studies.
Result: The LAS intake was about 780 mg/kg with the 1% diet, but there were no abnormalities in the body weight gains of the dams, or in the occurrence and maintenance of pregnancy. The values of the litter parameters did not differ from those of the controls and there was no evidence of teratogenicity. The numbers of offspring were rather low in the 1% group, and the weaning rate of 78.3% was lower than the 100% rate observed in the controls. However, there were no abnormalities in body weight gain, organ weights or functions in the offspring.
Source: European Commission 2000a; Tiba et al. 1976.
Reliability: (4) not assignable

21-MAR-2003 (12) (73)

Species: mouse **Sex:** female
Strain: ICR
Route of admin.: dermal
Exposure period: from day 6 through day 15 of pregnancy
Frequency of treatment: daily
Duration of test:
Doses: 0.03, 0.3, 3% (15, 150, and 1500 mg/kg bw d)
Control Group: yes
NOAEL Maternalt.: = 150 mg/kg bw
NOAEL Teratogen.: = 1500 mg/kg bw
Method: other: Areas of 4 x 4 cm on the backs of the mice were depilated and aqueous solutions of LAS were applied.
Year: **GLP:** no
Test substance: other TS: C10-14 LAS (CAS #69669-44-9); average alkyl chain length (based on LAS SIDS Consortium Survey, 2002) = C11.7; activity: 46.6%
Remark: Information as cited in the IUCLID Data Sheet and the IPCS document. This study represents the most appropriate NOAEL value identified by the Industry Coalition for the SIDS Assessment of LAS. The LAS Coalition reviewed seven developmental toxicity studies conducted on rats, mice and rabbits in which the test animals received LAS via the dermal route. While effects were observed at maternally toxic doses, no decreases in litter size, no changes in litter parameters, and no malformations or significant differences in skeletal defects were observed in these studies at dermal doses up to 1,500 mg/kg bwd. Note also that the NOAEL used in the risk assessment is derived from the repeated dose studies.
Result: The 3% group showed a clear decrease in the pregnancy rate (67.9%) when compared with a rate of 96.3% in the controls. However, there were no decreases in the litter size, and no changes in the litter parameters with the exception of a slight decrease in fetal body weight. There were no significant increases in the incidence of malformations in the fetuses.
Source: European Commission 2000a; Imahori et al. 1976.
Reliability: (4) not assignable
21-MAR-2003 (12) (24)

5.10 Other Relevant Information

Type:
Remark: None
11-OCT-2001

5.11 Experience with Human Exposure

Memo: LAS has been extensively studied and used for many years without significant incidents.
11-OCT-2001

(1) 49 CFR 173.1200 Appendix A. Method of testing corrosion to the skin.

(2) Buehler, E.V., Newmann, E.A., and King, W.R. 1971. Two year feeding and reproduction study in rats with linear alkylbenzene sulfonate (LAS). Toxicol. Appl. Pharmacol. 18:83-91.

(3) Cohen, L., Vergara, R., Moreno, A. and Berna, J.L. 1995. Influence of 2-phenyl alkane and telralin content on solubility and viscosity of linear alkylbenzene sulfonate. JAOCS 72:115-122.

(4) CONDEA Vista. 1995. Material Safety Data Sheet for VISTA SA-597L Sulfonic Acid, Revision No. 02/95, last revised 4/24/95.

(5) Cross, J. and Dekker, M. (ed.). 1977. Anionic surfactants: Chemical analysis, v. 8, p. 111-115.

(6) Deutsche Einheitsverfahren zur Wasser-, Abwasser- und Schlamm-untersuchung. L 11: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Kleinkrebse (Daphnien-Kurzzeittest). DIN 38412 Teil 11.

(7) Deutsche Einheitsverfahren zur Wasser-, Abwasser-, und Schlammuntersuchung. L 15: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische - Fischtest DIN 38412 Teil 15.

(8) Directive 84/449/EEC, B.14 mutagenicity. 1984. Salmonella typhimurium-reverse mutation assay.

(9) Directive 84/449/EEC, C.2. 1984. Acute toxicity for Daphnia.

(10) Douglas, M.T., Chanter, D.O., Pell, I.B., and Burney, G.M. 1986. A proposal for the reduction of animal numbers required for the acute toxicity to fish test (LC50 determination). Aquat. Toxicol. 8:243-249.

(11) Draize, J.H. 1965. Appraisal of the safety of chemicals in foods, drugs, and cosmetics-dermal toxicity. Association of Food and Drug Officials of the U.S., Topeka, Kansas Pp. 46-59.

(12) European Commission. 2000a. Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts. Year 2000 CD-ROM edition.

(13) Fedtke, N. 1991. Mutagenitatsprufung von Marlon AS 3 im in vivo mikrokerntest an der maus. Report No. MK-91/0026.

(14) Freitag, D., Ballhorn, L., Geyer, H., and Korte, F. 1985. An experimental method for the assessment of the behaviour of organic chemicals in the ecosphere by means of simple laboratory tests with C14 labelled chemicals. Chemosphere 14:1589-1616.

(15) Galassi et al. 1992. Water Res. 26:19-27 as cited in IUCLID. 1995. IUCLUD data sheet: dodecylbenzenesulfonic acid.

(15) Glaza, S.M. 1992. Dermal sensitization study of T-5474 in Guinea pigs – maximization test (EPA Guidelines). Hazleton Wisconin Labs, HWI Report Number 11203995.

(16) Hand, V.C. and Williams, G.K. 1987. Structure-activity relationships for sorption of linear alkylbenzenesulfonates. Environ. Sci. Technol. 21:370-373.

(17) Hempstock, C. 1998. NEOPELEX FS: Acute oral toxicity study in the rat - Acute toxic class method. SPL Project No. 140/854.

(18) HERA. 2002. HERA-LAS Human and Environmental Risk Assessment: Linear Alkylbenzene Sulphonates, LAS. CAS No. 68411-30-3, Draft #6, May 2002.

(19) Hoechst AG. 1988. Unveroffentlichte unters. ber. 88.0913. as cited in IUCLID. 1995. IUCLID data sheet: dodecylbenzenesulfonic acid.

(20) Hoechst AG. 1988. Unveroffentlichte unters. ber. 88.0925. as cited in IUCLID. 1995. IUCLID data sheet: dodecylbenzenesulfonic acid.

(21) Huels. 1993. Huels report No. DDA-21.

(22) Huntsman 2002. Report on the melting point analysis for NANSA HS 85/S. Attached technical bulletin dated 04-01-1994. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.

(23) Huntsman. 2002. Report of melting point analysis for NANSA HS 85/5. Cover memo from A. Ashworth to K.B. Sellstrom dated April 12, 2002.

(24) Imahori, A., Kinagawa, T. and Shiobara, S. 1976. Effects of linear alkyl benzene sulfonate (LAS) applied dermally to pregnant mice and their fetuses. Jpn. J. Public Health. 23:68-72 (in Japanese); cited in IPCS (1996); Environmental Health Criteria 169: Linear Aklylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

(25) Inoue, K., Shibata, T., Hamano, Y., Oda, Y., Kuwano, A., Yamamoto, H., Mitsuda, B. and Kunita, N. 1977. In vivo cytogenetic tests of some synthetic detergents in mice. Ann Res. Osaka Prefect Inst. Public Health. 8:17-24 (in Japanese); cited in: IPCS (1996); Environmental Health Criteria 169: Linear Aklylbenzene Sulfonates (LAS) and Related Compounds. WHO, Geneva, Switzerland.

(26) Inoue, K., Sunakawa, T., and Takayama. 1980. Studies of in vitro cell transformation and mutagenicity by surfactants and other compounds. Fd. Cosmet. Toxicol. 18:289-296.

(27) IUCLID. 1995. IUCLID data sheet: Benzenesulfonic acid, C10-16-alkyl derivatives.

(28) IUCLID. 1995. IUCLID data sheet: Dodecylbenzenesulphonic acid.

(29) Kinney, L.A. 1985. Approximate lethal concentrations (ALCs) by inhalation of sodium lauryl sulfate & sodium dodecylbenzene sulfonate. Dupont Haskell Laboratory Report No. 474-84.

(30) Knie, V.J., Halke, A., Juhnke, I., and Schiller, W. 1983. Ergebnisse der untersuchungen von chemischen stoffen mit vier biotests (Results of studies on chemical substances with four biotests). Deutsch Gewasserkundliche Mitteilungen 77-79.

(31) Kretchmar. 1972. Acute toxicity studies with XTW-1226. Report to Procter & Gamble Company, IBT No. A1717.

(32) Kurtin. 1994. Bestimmung der Auswirkungen von Marlon AS 3 auf das wachstum von Scendesmus subscipicatus 86.81.SAG. Report No. AW-371.

(33) Kurtin. 1994. Bestimmung der biologischen Abbaubarkeit von Marlon AS 3 im DOC-Die-Away test. Report No. DDA-79.

(34) Kurtin. 1994. Bestimmung der biologischen Abbaubarkeit von Marlon AS 3 im modifizierten coupled units-test. Report No. MCU-21.

(35) Kurtin. 1995. Bestimmung der auswirkungen von MARLON AS 3 auf das schwimmverhalten von Daphnic magna. Report No. DK-620.

(36) Kurtin. 1997. Bestimmung der akuten wirkungen von MARLON AS 3 gegenuber fischen. Report No. FK-1375.

(37) Kynoch, S.R. 1986a. Acute oral toxicity to rats: P-500 N-Na. Huntingdon Research Cener Report. No. 86546D/PEQ 7/AC.

(38) Kynoch, S.R. 1986b. Acute dermal toxicity to rats of P-500 N-Na. Huntingdon Research Center. Report No. 86718D/PEQ 8/AC.

(39) Leo, A.J. and Hansch, C. 1979. Substituent Constants for Correlation Analysis in Chemistry and Biology. J. Wiley & Sons, N.Y.

(40) Lide, D.R. 1990. Handbook of Chemistry and Physics. 71st Edition. CRC Press: Ann Arbor.

(41) Liggett, M.P. and Parcell, B.I. 1986a. Irritant effects on rabbit skin of P-500 N-Na. Huntingdon Research Center. Report No. 86400D/PEQ 9/SE.

(42) Liggett, M.P. and Parcell, B.I. 1986b. Irritant effects on the rabbit eye of P-500 N-Na. Huntingdon Research Center Report No. 86570D/PEQ 10/SE.

(43) Lyman, W.J. 1985. Environmental exposure from chemicals, V.I, p.31, Neely, W.B., and Blau, G.E., editors. CRC Press. Boca Raton.

(44) Magnusson, B. and Kligman, A.M. 1969. The identification of contact allergens by animal assay: The guinea pig maximization test. J. Invest. Dermatol. 52:268-276.

(45) Matsuura, T. and Smith, J.M. 1970. Kinetics of photodecomposition of dodecyl benzene sulfonate. Ing. Eng. Chem. Fund. 9:252-260.

(46) Murmann, P. 1984. Acute orale toxizitat von Marlon AS 3-Saure fur ratten. Report No. 0303.

(47) Murmann, P. 1984. Prufung der akuten augen- und schleimhautreizwirkung von Marlon AS 3-saure. Report No. 0305.

(48) Murmann, P. 1984. Prufung der akuten hautreizwirkung von Marlon AS 3-Saure. Report No. 0304.

(49) Murmann, P. 1984a. Akute orale Toxizitat von Marlon A 386 fur Ratten. Huels Report No. 0191.

(50) Noeller, C.R. 1966. Textbook of Organic Chemistry. 3rd Edition. W.B. Saunders Company: Philadelphia.

(51) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals 305E.

(52) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 401.

(53) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 404.

(54) Organisation for Economic Co-operation and Development (OECD). 1981. OECD guidelines for the testing of chemicals No. 405.

(55) Organisation for Economic Co-operation and Development (OECD). 1983. OECD guidelines for the testing of chemicals No. 474.

(56) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals No. 201.

(57) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals No. 202.

(58) Organisation for Economic Co-operation and Development (OECD). 1984. OECD guidelines for the testing of chemicals, No. 203.

(59) Organisation for Economic Co-operation and Development (OECD). 1987. OECD guidelines for the testing of chemicals, No. 401.

(60) Organisation for Economic Co-operation and Development (OECD). 1992. OECD guidelines for the testing of chemicals, No. 203.

(61) Organisation for Economic Co-operation and Development (OECD). 1992. OECD guidelines for the testing of chemicals, No. 301B.

(62) Organisation for Economic Co-operation and Development (OECD). 1995. OECD guidelines for the testing of chemicals, No. 202.

(63) Procter & Gamble. 1991. AT/17.

(64) RBM. 1985. Test di sensibilizzazione cutanea nella cavia. RBM Exp. No. 2076.

(65) Roberts, D.W. 1991. QSAR issues in aquatic toxicity of surfactants. Sci. Total Environ. 109/110:557-568.

(66) Rose, G.P. 1983. Toxicology of detergents: The skin sensitizing potential of Dobanic acid 103. Group research report SBGR.83.383.

(67) Schoberl, P. 1991. Coupling the OECD confirmatory-test with continuous ecotoxicity tests. Communication 1: Modification of the OECD confirmatory test (sewage treatment plant simulation model). Tenside Surfactants Detergents 6.

(68) Schoeberl, P. 1993a. Bestimmung der Mutagenitat von Marlon A 390 im Salmonella/Sauger-Mikrosomen-Mutagenitatstest nach Ames. Huels Final Report No. AM-93/12.

(69) Stepan Company. Biotic degradation (modified Sturm test) evaluation, in an aqueous medium, of the "ultimate" biodegradability of substances: 1736-1A, 1736-1B, 1736-1C, 1736-1D, 1736-1E. Ineris-Study 16 BF 53.

(70) Stephenson, R.R. 1981. Dobanic acid 102: Acute toxicity to Salmo gairdneri, Daphnia magna, and Selenstrum capricornutum. Group research preport SBGR.81.083.

(71) Thompson, G.W. 1980. D.O.T. skin corrosivity-method, summary for Bio-Soft S-100. Raltech Scientific Services. Lab Study No. 793159.

(72) Thompson, P.W. 1998. NEOPELEX FS: Reverse mutation assay "Ames test" using Salmonella typhimurium strains TA 98 and TA 100 - single experiment. SLP Project No. 140/855.

(73) Tiba, S., Shiobara, S., Imahori, A. and Kitagawa, T. 1976. Effects of linear alkylbenzene sulfonate on dam, fetus and newborn rat. J. Food Hyg. Soc. Jpn. 17:66-71. (In Japanese); cited in IPCS. 1996. Environmental Health Criteria 169: Linear Alkylbenzene Sulfonates and Related Compounds. World Health Organization, Geneva, Switzerland. Original article in Japanese.

(74) Tolls, J., Haller, M., DeGraaf, I., Thijssenk, M.A.T.C., and Sijm, D.T.H.M. 1997. Bioconcentration of LAS: Experimental determination and extrapolation to environmental mixtures. Environ. Sci. Technol. 31:3426-3431.

(75) USEPA 1985.

(76) USEPA. 2000. EpiSuite Estimation Software V.3.10. US Environmental Protection Agency.

(77) van de Plassche, E.J., DeBruijn, J.H.M., Stephenson, R.R., Marshall, S.J., Feijtel, T.C.J., and Belanger, S.E. 1999. Predicted no-effect concentrations and risk characterization of four surfactants: Linear alkyl benzene sulfonate, alcohol ethoxylates, alcohol ethoxylated sulfates, and soap. Environ. Toxicol. Chem. 18: 2653-2663.

(78) Verge, C. and Moreno, A. 1996. Toxicity of anionic surfactants to green microalgae "Scenedesmus subspicatus" and "Selenastrum capricornutum". Tenside Surf. Det. 33:166-168.

(79) Verge, C. and Moreno, A. 2000. Effects of anionic surfactant on Daphnia magna. Tenside Surf. Det. 37:172-175.

(80) Verschueren, K. 1996. Handbook of Environmental Data on Organic Chemicals, Third Edition. New York: John Wiley & Sons, Inc.

(81) Yoneyama, M., Mabuchi, Y., Ikawa, M., Kobayashi, H. and Ichikawa, H. 1976. Subacute toxicity of linear alkylbenzene sulfonate. Ann. Rep. Tokyo Metr. Res. Lab. Public Health 27:105-112 (in Japanese); cited in: IPCS (1996); Environmental Heath Criteria 169: Linear Aklylbenzene Sulfonates (LAS) and Related Compounds. WHO Geneva, Switzerland.

7.1 Risk Assessment

Memo: See LAB sulfonic acids assessment plan.
21-MAR-2003